GREEN CHEMISTRY EXPERT SYSTEM (GCES)

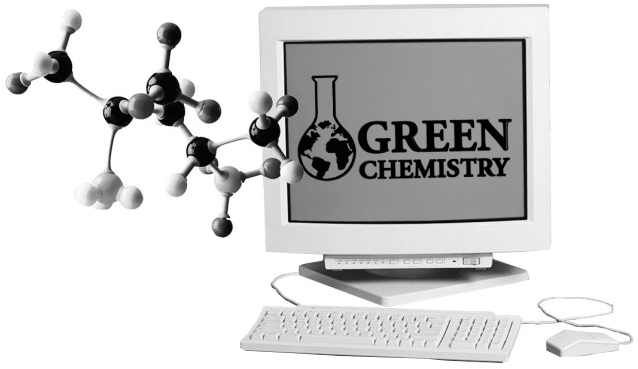
What is GCES?

GCES is a stand-alone program designed to help the user design a safer chemical and chemical process. It comes pre-loaded with much of the information needed to carry out this task. It contains context-sensitive help screens to explain options and numerous prompts to confirm selected operations or to request additional information. It includes extensive system documentation.

How Does GCES Assist Users?

- Identifies opportunities to eliminate or reduce the use or production of hazardous substances during chemical manufacture.
- Suggests molecular modifications to minimize toxicity and provides techniques that might reduce hazards to health and the environment.
- Presents technical information on green synthesis, solvent systems, reaction conditions, and chemical products.
- Provides a database of useful green chemistry references.

The GCES features are contained in five modules.



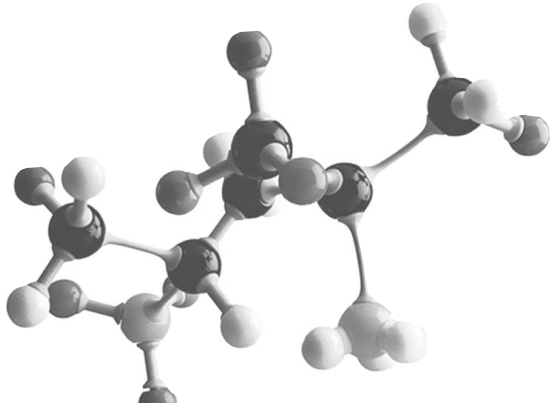
SMART Module

The Synthetic Methodology Assessment for Reduction Techniques (SMART) module began as an internal EPA program. Under the SMART program, EPA assesses manufacturing methods and subsequently recommends alternative approaches to reduce sources of pollution prior to commercial production of a new chemical substance.

The SMART module automates the calculations used in these assessments. It quantifies and sorts the hazardous substances used in or generated by a chemical reaction, based on information entered by the user and a built-in database of more than 60,000 chemicals. The SMART module initially provides the user with a graphical output classifying each chemical into one of four hazard tiers and identifying the amount of waste the reaction generates relative to the amount of product recovered. The SMART module then points the user to other GCES modules for information on developing a green alternative.

Green Synthetic Reactions Module

This module provides technical information on green synthetic reactions. It is searchable by keywords and may be used to identify a reaction to replace a specific hazardous reactant or byproduct. Its also contains full reference citations.



Designing Safer Chemicals Module

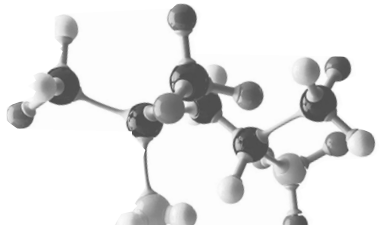
The Designing Safer Chemicals module helps users understand and predict structural modifications that result in safer chemicals. The Chemical Classes section contains a brief description of the toxicological concerns for a variety of structural classes, followed by descriptions of specific molecular modifications that are expected to minimize toxicity. A series of linked questions guides the user through suggested modifications. The Chemical Characteristics section provides links to external programs allowing estimation of persistence, bioaccumulation, and aquatic toxicity.

Green Solvents/Reaction Conditions Module

This module discusses alternatives to traditional organic solvents. Overviews of solventless conditions, aqueous systems, supercritical/dense phase fluids, immobilized solvents, and ionic liquids are provided along with key references. A fully-searchable database of physicochemical properties of more than 600 solvents is included to assist in finding green replacement solvents.

Green Chemistry References Module

This module contains useful references for a variety of green chemistry topics. It is text-searchable in all fields, including the abstract field; references are grouped into categories to allow users to search or browse a subset of the module. Several hundred references are included and users can add additional references to this module.



System Requirements

Windows 3.x, Windows 95, or Windows 98

20 MB free hard disk space for complete installation *or*
5 MB free hard disk space for minimal installation and 15 MB on another drive.

GCES is available for download from the Green Chemistry web site at www.epa.gov/greenchemistry.

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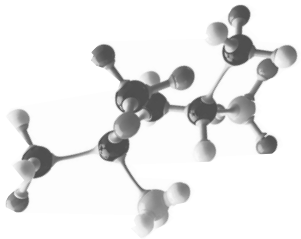

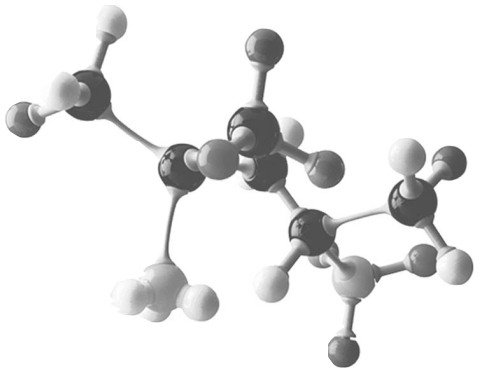

EPA
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United States Environmental Protection Agency
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www.epa.gov/greenchemistry
Office of Pollution Prevention and Toxics (7406)

EPA

Green Chemistry Expert System

Version 0.99

The Green Chemistry Expert System (GCES) allows users to build a green chemical process, design a green chemical, or survey the field of green chemistry. Green chemistry is the design of chemical products and processes that reduce or eliminate the use or generation of hazardous substances. This new approach to pollution prevention is the central focus of the U.S. Environmental Protection Agency's (EPA's) Green Chemistry Program, an initiative under the EPA Design for the Environment (DfE) Program.

Green Chemistry Program
Industrial Chemistry Branch
Economics, Exposure, and Technology Division
Office of Pollution Prevention and Toxics

Design for the Environment U.S. EPA

GREEN CHEMISTRY